Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 11:12 PM EDT

PDB ID	:	1I09
Title	:	STRUCTURE OF GLYCOGEN SYNTHASE KINASE-3 (GSK3B)
Authors	:	Ter Haar, E.; Coll, J.T.; Jain, J.
Deposited on	:	2001-01-29
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

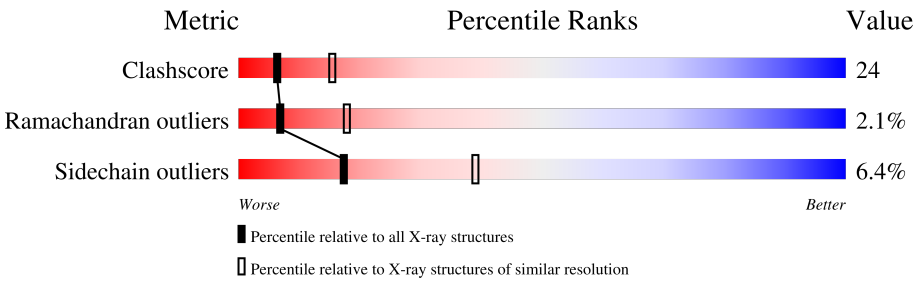
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	420	48% 29% • 20%
1	B	420	47% 29% 5% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	421	-	-	X	-
2	PO4	B	421	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5304 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

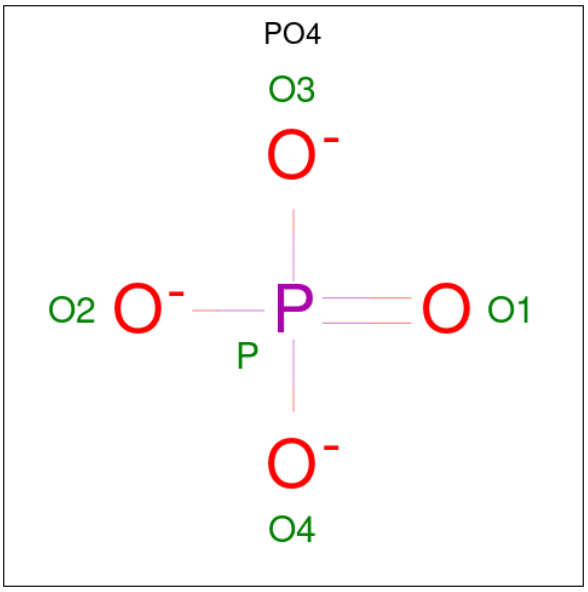
- Molecule 1 is a protein called GLYCOGEN SYNTHASE KINASE-3 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2615	1678	447	478	12	77	0	0
1	B	341	2623	1691	435	486	11	57	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	LEU	HIS	SEE REMARK 999	UNP P49841
B	350	LEU	HIS	SEE REMARK 999	UNP P49841

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
			Total	O	P		
2	B	1	5	4	1	0	0
			Total	O	P		
2	B	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	23	23	23	0	0
			Total	O		
3	B	23	23	23	0	0

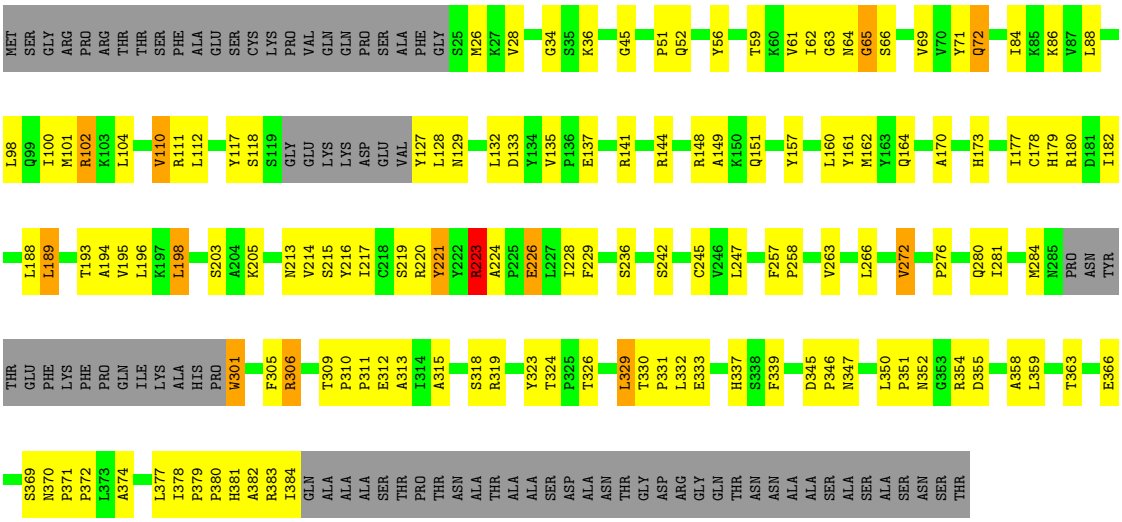
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

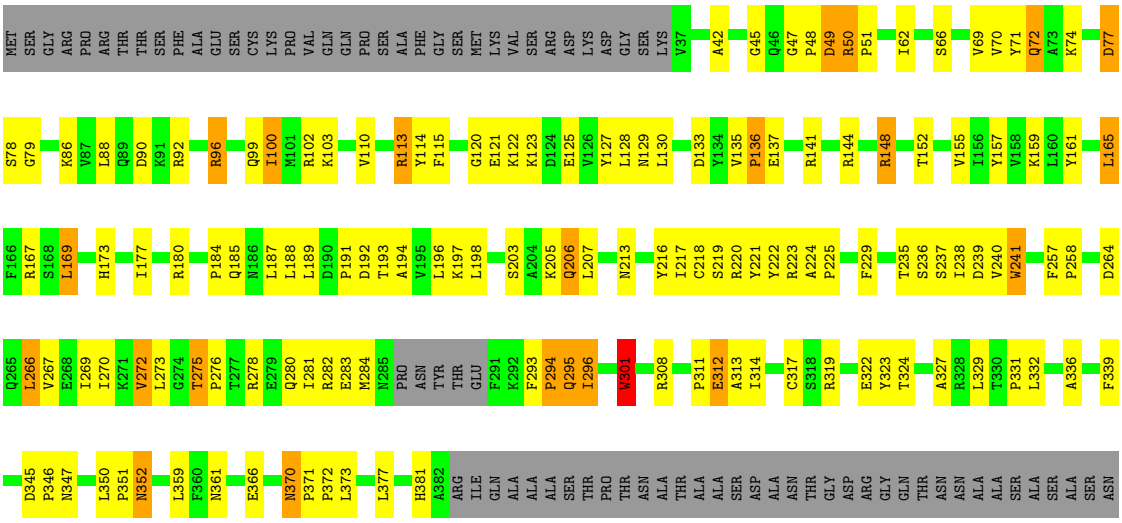
• Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA

Chain A: 48% 29% • 20%



• Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA

Chain B: 47% 29% 5% 19%



SER
THR

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.27Å 86.72Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (48.30-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.242 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5304	wwPDB-VP
Average B, all atoms ($Å^2$)	39.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.53	1/2675 (0.0%)	0.88	7/3642 (0.2%)
1	B	0.53	2/2688 (0.1%)	0.78	4/3671 (0.1%)
All	All	0.53	3/5363 (0.1%)	0.83	11/7313 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	TRP	NE1-CE2	8.74	1.49	1.37
1	B	241	TRP	NE1-CE2	8.72	1.48	1.37
1	B	301	TRP	NE1-CE2	8.61	1.48	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	223	ARG	NE-CZ-NH2	-20.68	109.96	120.30
1	A	223	ARG	NE-CZ-NH1	17.02	128.81	120.30
1	B	100	ILE	CA-CB-CG1	8.05	126.30	111.00
1	A	223	ARG	CG-CD-NE	7.66	127.89	111.80
1	B	123	LYS	O-C-N	-6.99	111.51	122.70
1	A	221	TYR	O-C-N	-6.84	111.75	122.70
1	A	72	GLN	O-C-N	-6.17	112.84	122.70
1	B	308	ARG	CB-CA-C	-5.96	98.49	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	223	ARG	CB-CG-CD	-5.77	96.59	111.60
1	B	295	GLN	O-C-N	-5.77	113.47	122.70
1	A	223	ARG	CD-NE-CZ	5.27	130.98	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2615	0	2595	114	0
1	B	2623	0	2559	129	0
2	A	10	0	0	3	0
2	B	10	0	0	4	0
3	A	23	0	0	0	0
3	B	23	0	0	0	0
All	All	5304	0	5154	242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PRO:HB2	1:B:284:MET:CE	1.60	1.29
1:B:225:PRO:CB	1:B:284:MET:HE3	1.66	1.24
1:B:216:TYR:O	1:B:216:TYR:CD1	2.06	1.09
1:A:216:TYR:HD1	1:A:216:TYR:O	1.40	1.05
1:A:215:SER:O	1:A:223:ARG:NH2	1.89	1.04
1:A:64:ASN:O	1:A:65:GLY:O	1.79	1.01
1:A:216:TYR:O	1:A:216:TYR:CD1	2.21	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ARG:O	1:B:281:ILE:HG22	1.69	0.91
1:B:216:TYR:O	1:B:216:TYR:HD1	1.51	0.91
1:B:283:GLU:OE1	1:B:324:THR:HG23	1.72	0.90
1:A:128:LEU:HD12	1:A:129:ASN:H	1.37	0.89
1:B:370:ASN:HD22	1:B:372:PRO:HD2	1.43	0.84
1:A:56:TYR:HE1	1:A:59:THR:HG21	1.43	0.83
1:A:149:ALA:O	1:A:151:GLN:HG3	1.79	0.83
1:A:56:TYR:HE1	1:A:59:THR:CG2	1.91	0.82
1:A:284:MET:HE3	1:A:323:TYR:CD2	2.15	0.81
1:A:284:MET:CE	1:A:323:TYR:HD2	1.93	0.81
1:A:284:MET:CE	1:A:323:TYR:CD2	2.63	0.80
1:B:229:PHE:CD2	1:B:284:MET:HE2	2.17	0.79
1:A:128:LEU:HD12	1:A:129:ASN:N	1.98	0.78
1:A:337:HIS:HD2	1:A:339:PHE:H	1.32	0.77
1:B:62:ILE:HG21	1:B:72:GLN:HB3	1.66	0.77
1:B:275:THR:HG22	1:B:276:PRO:HD2	1.68	0.75
1:B:370:ASN:ND2	1:B:372:PRO:HD2	2.00	0.75
1:B:120:GLY:HA2	1:B:127:TYR:CE1	2.23	0.74
1:B:205:LYS:HD2	2:B:421:PO4:O2	1.88	0.74
1:B:225:PRO:HB2	1:B:284:MET:HE3	0.79	0.74
1:A:28:VAL:HG21	1:A:36:LYS:HE3	1.70	0.73
1:A:56:TYR:CE1	1:A:59:THR:CG2	2.71	0.73
1:A:118:SER:O	1:A:127:TYR:HA	1.90	0.71
1:B:219:SER:O	1:B:223:ARG:HG3	1.91	0.71
1:B:100:ILE:HG21	1:B:177:ILE:HD13	1.73	0.69
1:B:203:SER:HB3	1:B:217:ILE:HD11	1.75	0.69
1:B:229:PHE:HD2	1:B:284:MET:HE2	1.56	0.68
1:B:370:ASN:HD22	1:B:370:ASN:C	1.98	0.67
1:A:62:ILE:HD13	1:A:72:GLN:HB2	1.76	0.67
1:B:319:ARG:HB3	1:B:329:LEU:HD13	1.77	0.66
1:B:278:ARG:O	1:B:281:ILE:CG2	2.43	0.66
1:B:312:GLU:CD	1:B:312:GLU:H	1.99	0.66
1:A:337:HIS:CD2	1:A:339:PHE:H	2.13	0.66
1:B:120:GLY:HA3	1:B:125:GLU:HG3	1.76	0.66
1:B:219:SER:O	1:B:223:ARG:CG	2.45	0.65
1:A:101:MET:CE	1:A:132:LEU:HD21	2.27	0.65
1:A:228:ILE:HG21	1:A:266:LEU:CD1	2.25	0.65
1:B:100:ILE:CG2	1:B:177:ILE:HD13	2.25	0.65
1:A:228:ILE:HG21	1:A:266:LEU:HD13	1.79	0.65
1:B:275:THR:HG22	1:B:276:PRO:CD	2.26	0.65
1:B:180:ARG:HD3	1:B:203:SER:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PHE:CE2	1:B:284:MET:CE	2.80	0.64
1:A:62:ILE:HG13	1:A:63:GLY:N	2.12	0.64
1:A:56:TYR:CE1	1:A:59:THR:HG22	2.33	0.62
1:B:42:ALA:HB1	1:B:114:TYR:HB3	1.81	0.62
1:B:196:LEU:HD23	1:B:197:LYS:N	2.14	0.62
1:A:205:LYS:NZ	1:A:213:ASN:OD1	2.23	0.62
1:A:346:PRO:HB3	1:A:381:HIS:CD2	2.34	0.61
1:A:358:ALA:O	1:A:359:LEU:HD23	2.01	0.61
1:A:324:THR:HG22	1:A:326:THR:HG22	1.82	0.61
1:A:280:GLN:NE2	1:A:323:TYR:CD1	2.68	0.61
1:B:155:VAL:O	1:B:159:LYS:HG3	2.00	0.60
1:A:193:THR:OG1	1:A:195:VAL:HG13	2.02	0.59
1:A:257:PHE:HE1	1:A:272:VAL:HG21	1.67	0.59
1:B:115:PHE:HA	1:B:129:ASN:O	2.01	0.59
1:B:165:LEU:HD22	1:B:169:LEU:HD22	1.85	0.59
1:A:219:SER:O	1:A:223:ARG:HG2	2.03	0.59
1:A:173:HIS:ND1	2:A:422:PO4:O3	2.35	0.58
1:B:345:ASP:OD2	1:B:347:ASN:HB2	2.04	0.58
1:B:88:LEU:HA	1:B:127:TYR:CD2	2.39	0.57
1:A:117:TYR:CE1	1:A:128:LEU:HD13	2.40	0.56
1:B:229:PHE:CD2	1:B:284:MET:CE	2.88	0.56
1:A:332:LEU:HD22	1:A:377:LEU:HD11	1.87	0.56
1:B:225:PRO:HD3	1:B:241:TRP:CZ2	2.41	0.56
1:B:113:ARG:NE	1:B:133:ASP:OD2	2.36	0.56
1:A:179:HIS:O	1:A:180:ARG:HB2	2.06	0.55
1:B:272:VAL:HG22	1:B:273:LEU:HD23	1.89	0.55
1:A:45:GLY:HA3	1:A:112:LEU:O	2.06	0.55
1:A:284:MET:HE1	1:A:323:TYR:CD2	2.39	0.55
1:B:283:GLU:HG2	1:B:283:GLU:O	2.06	0.55
1:A:100:ILE:HG23	1:A:177:ILE:HD13	1.90	0.54
1:A:101:MET:HE3	1:A:132:LEU:HD21	1.89	0.54
1:B:157:TYR:OH	1:B:351:PRO:HG2	2.07	0.54
1:B:157:TYR:OH	1:B:351:PRO:CG	2.54	0.54
1:A:263:VAL:HG21	1:B:217:ILE:HD12	1.90	0.54
1:A:350:LEU:HB3	1:A:351:PRO:HD2	1.90	0.54
1:B:264:ASP:O	1:B:267:VAL:HG22	2.07	0.54
1:B:217:ILE:HG23	1:B:218:CYS:N	2.21	0.54
1:B:62:ILE:CG2	1:B:72:GLN:HB3	2.38	0.53
1:B:257:PHE:CE1	1:B:269:ILE:HA	2.44	0.53
1:B:135:VAL:HB	1:B:188:LEU:HD13	1.89	0.53
1:A:64:ASN:C	1:A:65:GLY:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TYR:CD1	1:A:216:TYR:C	2.82	0.53
1:B:113:ARG:HH11	1:B:113:ARG:HB3	1.74	0.53
1:B:121:GLU:N	1:B:125:GLU:OE2	2.42	0.53
1:A:101:MET:HE1	1:A:132:LEU:HD21	1.90	0.53
1:B:270:ILE:HG23	1:B:275:THR:HA	1.90	0.53
1:A:276:PRO:HA	1:A:280:GLN:NE2	2.24	0.52
1:B:196:LEU:HD23	1:B:196:LEU:C	2.29	0.52
1:A:301:TRP:CZ3	1:A:305:PHE:HE1	2.28	0.52
1:A:26:MET:HE1	1:A:118:SER:OG	2.09	0.52
1:A:71:TYR:HB2	1:A:84:ILE:HB	1.92	0.52
1:B:122:LYS:H	1:B:125:GLU:CD	2.13	0.52
1:A:280:GLN:NE2	1:A:323:TYR:HD1	2.06	0.52
1:A:193:THR:O	1:A:194:ALA:HB3	2.09	0.52
1:A:381:HIS:HA	1:A:384:ILE:HD12	1.92	0.51
1:A:56:TYR:CE1	1:A:59:THR:HG21	2.32	0.51
1:B:280:GLN:NE2	1:B:323:TYR:CD2	2.77	0.51
1:B:229:PHE:HE2	1:B:284:MET:CE	2.23	0.51
1:B:173:HIS:CE1	1:B:236:SER:HB3	2.46	0.51
1:B:350:LEU:C	1:B:352:ASN:H	2.13	0.51
1:B:350:LEU:C	1:B:352:ASN:N	2.61	0.51
1:A:170:ALA:HB2	1:A:331:PRO:HB2	1.92	0.51
1:A:363:THR:OG1	1:A:366:GLU:HG3	2.10	0.51
1:B:69:VAL:CG1	1:B:70:VAL:N	2.74	0.50
1:A:137:GLU:OE2	1:A:141:ARG:NE	2.44	0.50
1:A:324:THR:CG2	1:A:326:THR:HG22	2.41	0.50
1:B:69:VAL:HG12	1:B:70:VAL:N	2.25	0.50
1:B:332:LEU:HG	1:B:373:LEU:HD23	1.94	0.50
1:A:26:MET:CE	1:A:118:SER:OG	2.59	0.50
1:B:86:LYS:HE2	1:B:127:TYR:CD1	2.47	0.50
1:B:122:LYS:H	1:B:125:GLU:CG	2.25	0.50
1:A:301:TRP:HA	1:A:301:TRP:CE3	2.47	0.50
1:A:370:ASN:OD1	1:A:372:PRO:HG2	2.12	0.50
1:B:205:LYS:CD	2:B:421:PO4:O2	2.59	0.49
1:B:128:LEU:HG	1:B:130:LEU:CD1	2.42	0.49
1:B:137:GLU:OE2	1:B:141:ARG:NH1	2.44	0.49
1:B:167:ARG:HD2	1:B:366:GLU:OE2	2.13	0.49
1:B:370:ASN:ND2	1:B:370:ASN:C	2.65	0.49
1:A:219:SER:O	1:A:223:ARG:CG	2.61	0.49
1:B:120:GLY:HA2	1:B:127:TYR:HE1	1.74	0.49
1:A:224:ALA:HB1	1:A:226:GLU:OE2	2.13	0.49
1:B:229:PHE:CE2	1:B:284:MET:HE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:O	1:A:310:PRO:C	2.49	0.49
1:B:216:TYR:CD1	1:B:216:TYR:C	2.85	0.49
1:B:224:ALA:HA	1:B:241:TRP:CD1	2.47	0.49
1:A:330:THR:HG23	1:A:333:GLU:OE1	2.12	0.49
1:B:294:PRO:O	1:B:296:ILE:N	2.46	0.49
1:B:370:ASN:HB3	1:B:373:LEU:HD22	1.95	0.49
1:B:278:ARG:C	1:B:281:ILE:HG22	2.31	0.48
1:A:371:PRO:HB2	1:A:372:PRO:CD	2.43	0.48
1:B:301:TRP:CE3	1:B:301:TRP:HA	2.49	0.48
1:B:50:ARG:HE	1:B:50:ARG:HA	1.77	0.48
1:A:301:TRP:HZ3	1:A:305:PHE:CE1	2.32	0.48
1:B:49:ASP:C	1:B:51:PRO:HD3	2.35	0.47
1:B:103:LYS:HG3	1:B:103:LYS:O	2.13	0.47
1:A:182:ILE:CD1	1:A:198:LEU:HD11	2.43	0.47
1:A:301:TRP:CZ3	1:A:305:PHE:CE1	3.02	0.47
1:A:160:LEU:HD11	1:A:350:LEU:CD2	2.44	0.47
1:B:313:ALA:HB2	1:B:339:PHE:CE1	2.49	0.47
1:A:28:VAL:HG21	1:A:36:LYS:CE	2.42	0.47
1:A:161:TYR:CZ	1:A:189:LEU:HD12	2.50	0.47
1:A:281:ILE:O	1:A:284:MET:N	2.44	0.47
1:A:306:ARG:O	1:A:309:THR:HG22	2.15	0.47
1:B:312:GLU:OE1	1:B:312:GLU:N	2.48	0.47
1:B:48:PRO:O	1:B:50:ARG:N	2.48	0.46
1:A:221:TYR:CD1	1:A:258:PRO:HA	2.50	0.46
1:A:214:VAL:HG13	2:A:421:PO4:O1	2.15	0.46
1:A:180:ARG:HD3	1:A:203:SER:O	2.16	0.46
1:B:71:TYR:N	1:B:71:TYR:CD1	2.84	0.46
1:A:62:ILE:CG2	1:A:72:GLN:HB2	2.46	0.45
1:A:135:VAL:HB	1:A:188:LEU:HB3	1.98	0.45
1:A:379:PRO:O	1:A:382:ALA:HB3	2.16	0.45
1:B:266:LEU:O	1:B:270:ILE:HG13	2.17	0.45
1:A:319:ARG:HA	1:A:319:ARG:HH11	1.82	0.45
1:B:238:ILE:HG13	1:B:239:ASP:N	2.31	0.45
1:B:191:PRO:HG2	1:B:192:ASP:H	1.82	0.45
1:A:345:ASP:OD1	1:A:347:ASN:N	2.42	0.45
1:A:381:HIS:HA	1:A:384:ILE:CD1	2.47	0.45
1:B:90:ASP:OD1	1:B:92:ARG:N	2.49	0.45
1:B:144:ARG:O	1:B:148:ARG:HB2	2.17	0.45
1:A:306:ARG:O	1:A:309:THR:CG2	2.64	0.45
1:B:136:PRO:HG2	1:B:137:GLU:H	1.82	0.45
1:A:64:ASN:O	1:A:65:GLY:C	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:C	1:A:352:ASN:N	2.67	0.44
1:B:45:GLY:O	1:B:102:ARG:HD2	2.17	0.44
1:B:72:GLN:HE21	1:B:72:GLN:HB2	1.54	0.44
1:A:110:VAL:CG1	1:A:188:LEU:HD12	2.47	0.44
1:A:160:LEU:O	1:A:164:GLN:HG3	2.17	0.44
1:B:229:PHE:HE2	1:B:284:MET:HE1	1.82	0.44
1:A:228:ILE:HG21	1:A:266:LEU:HD11	1.99	0.44
1:A:144:ARG:O	1:A:148:ARG:HG2	2.18	0.44
1:A:196:LEU:C	1:A:196:LEU:HD23	2.37	0.44
1:A:312:GLU:N	1:A:312:GLU:CD	2.71	0.44
1:A:378:ILE:O	1:A:383:ARG:NH1	2.50	0.44
1:B:219:SER:O	1:B:223:ARG:HG2	2.18	0.44
1:B:346:PRO:HB3	1:B:381:HIS:CD2	2.52	0.43
1:B:74:LYS:HE2	1:B:79:GLY:HA2	2.00	0.43
1:B:96:ARG:O	1:B:99:GLN:HB3	2.18	0.43
1:B:207:LEU:HD22	1:B:213:ASN:ND2	2.34	0.43
1:B:311:PRO:O	1:B:314:ILE:N	2.52	0.43
1:A:56:TYR:CD1	1:A:59:THR:HG22	2.53	0.43
1:B:217:ILE:CG2	1:B:218:CYS:N	2.81	0.43
1:A:371:PRO:N	1:A:372:PRO:HD2	2.34	0.43
1:B:100:ILE:O	1:B:100:ILE:HG22	2.18	0.43
1:B:235:THR:O	1:B:238:ILE:HG12	2.18	0.43
1:B:281:ILE:HG23	1:B:282:ARG:N	2.33	0.43
1:A:315:ALA:O	1:A:318:SER:OG	2.29	0.43
1:B:157:TYR:OH	1:B:351:PRO:HG3	2.18	0.43
1:A:157:TYR:OH	1:A:351:PRO:HG3	2.19	0.43
1:B:96:ARG:HG3	1:B:96:ARG:HH11	1.84	0.42
1:B:205:LYS:HG2	1:B:206:GLN:N	2.34	0.42
1:B:324:THR:HG22	1:B:327:ALA:N	2.33	0.42
1:A:178:CYS:SG	1:A:236:SER:HA	2.59	0.42
1:B:77:ASP:OD1	1:B:78:SER:N	2.48	0.42
1:B:185:GLN:CD	1:B:185:GLN:H	2.23	0.42
1:B:370:ASN:CG	1:B:373:LEU:HD13	2.39	0.42
1:A:100:ILE:O	1:A:104:LEU:HD13	2.19	0.42
1:B:319:ARG:HB3	1:B:329:LEU:CD1	2.46	0.42
1:B:331:PRO:HD3	2:B:422:PO4:O3	2.19	0.42
1:A:374:ALA:HA	1:A:377:LEU:HB2	2.01	0.42
1:B:135:VAL:HA	1:B:136:PRO:HD2	1.84	0.42
1:A:379:PRO:HA	1:A:380:PRO:HD3	1.91	0.42
1:B:161:TYR:CZ	1:B:189:LEU:HD22	2.55	0.42
1:B:193:THR:O	1:B:194:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD23	1:B:373:LEU:HD22	2.01	0.42
1:A:352:ASN:ND2	1:A:354:ARG:HD3	2.34	0.42
1:A:161:TYR:CE1	1:A:189:LEU:HD12	2.55	0.41
1:A:128:LEU:CD1	1:A:129:ASN:N	2.78	0.41
1:A:162:MET:HG3	1:A:247:LEU:HD13	2.02	0.41
1:A:313:ALA:HB2	1:A:339:PHE:CE1	2.55	0.41
1:B:218:CYS:HB3	1:B:223:ARG:HG2	2.02	0.41
1:B:110:VAL:HG12	1:B:198:LEU:O	2.20	0.41
1:B:206:GLN:HE21	1:B:206:GLN:HB3	1.46	0.41
1:A:257:PHE:HE1	1:A:272:VAL:CG2	2.33	0.41
1:B:371:PRO:HB2	1:B:372:PRO:HD3	2.03	0.41
1:A:86:LYS:HA	1:A:128:LEU:O	2.20	0.41
1:B:96:ARG:HG3	1:B:96:ARG:NH1	2.36	0.41
1:B:205:LYS:CE	2:B:421:PO4:O2	2.69	0.41
1:B:237:SER:O	1:B:240:VAL:HB	2.20	0.41
1:A:319:ARG:HB3	1:A:329:LEU:HD13	2.02	0.41
1:B:88:LEU:HA	1:B:127:TYR:HD2	1.84	0.41
1:A:214:VAL:HG22	2:A:421:PO4:O1	2.21	0.41
1:A:242:SER:O	1:A:245:CYS:HB2	2.21	0.41
1:B:221:TYR:CD1	1:B:258:PRO:HA	2.56	0.41
1:B:225:PRO:HD3	1:B:241:TRP:CE2	2.56	0.41
1:A:229:PHE:HE2	1:A:284:MET:SD	2.44	0.41
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.69	0.40
1:A:332:LEU:HD22	1:A:377:LEU:CD1	2.50	0.40
1:A:98:LEU:O	1:A:102:ARG:HB2	2.22	0.40
1:B:167:ARG:NH2	1:B:361:ASN:OD1	2.50	0.40
1:B:312:GLU:CD	1:B:312:GLU:N	2.71	0.40
1:A:111:ARG:HB2	1:A:133:ASP:OD2	2.22	0.40
1:B:184:PRO:HD3	1:B:222:TYR:CE2	2.56	0.40
1:B:336:ALA:HB2	1:B:377:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/420 (79%)	302 (91%)	25 (8%)	5 (2%)	10	26
1	B	337/420 (80%)	298 (88%)	30 (9%)	9 (3%)	5	12
All	All	669/840 (80%)	600 (90%)	55 (8%)	14 (2%)	7	18

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLY
1	B	49	ASP
1	B	294	PRO
1	A	34	GLY
1	A	61	VAL
1	B	220	ARG
1	B	295	GLN
1	A	51	PRO
1	A	220	ARG
1	B	47	GLY
1	B	136	PRO
1	B	77	ASP
1	B	296	ILE
1	B	293	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/364 (78%)	268 (95%)	15 (5%)	22	48
1	B	281/364 (77%)	260 (92%)	21 (8%)	13	31
All	All	564/728 (78%)	528 (94%)	36 (6%)	17	39

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	66	SER
1	A	69	VAL
1	A	88	LEU
1	A	102	ARG
1	A	110	VAL
1	A	189	LEU
1	A	198	LEU
1	A	217	ILE
1	A	226	GLU
1	A	272	VAL
1	A	306	ARG
1	A	329	LEU
1	A	355	ASP
1	A	369	SER
1	B	50	ARG
1	B	66	SER
1	B	72	GLN
1	B	96	ARG
1	B	113	ARG
1	B	148	ARG
1	B	152	THR
1	B	165	LEU
1	B	169	LEU
1	B	187	LEU
1	B	206	GLN
1	B	266	LEU
1	B	272	VAL
1	B	275	THR
1	B	301	TRP
1	B	312	GLU
1	B	317	CYS
1	B	322	GLU
1	B	352	ASN
1	B	359	LEU
1	B	370	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	108	ASN
1	A	129	ASN

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	206	GLN
1	A	280	GLN
1	A	337	HIS
1	B	64	ASN
1	B	72	GLN
1	B	99	GLN
1	B	108	ASN
1	B	254	GLN
1	B	280	GLN
1	B	370	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	B	421	-	4,4,4	2.18	3 (75%)	6,6,6	0.75	0
2	PO4	A	422	-	4,4,4	1.54	1 (25%)	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	421	-	4,4,4	2.33	3 (75%)	6,6,6	0.80	0
2	PO4	B	422	-	4,4,4	1.28	0	6,6,6	0.46	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	421	PO4	P-O1	-2.82	1.44	1.50
2	A	421	PO4	P-O3	-2.56	1.47	1.54
2	B	421	PO4	P-O2	-2.50	1.47	1.54
2	B	421	PO4	P-O1	-2.45	1.45	1.50
2	A	421	PO4	P-O2	-2.42	1.47	1.54
2	B	421	PO4	P-O3	-2.39	1.47	1.54
2	A	422	PO4	P-O3	-2.07	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	421	PO4	3	0
2	A	422	PO4	1	0
2	A	421	PO4	2	0
2	B	422	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.